Probing Pauli Blocking Factors in Quantum Pumps with Broken Time-Reversal Symmetry

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A recently demonstrated quantum electron pump is discussed within the framework of photon-assisted tunneling. Due to lack of time-reversal symmetry, different results are obtained for the pump current depending on whether or not final-state Pauli blocking factors are used when describing the tunneling process. Whilst in both cases the current depends quadratically on the driving amplitude for moderate pumping, a marked difference is predicted for the temperature dependence. With blocking factors the pump current decreases roughly linearly with temperature until $k_{\mathrm{B}}T \approx \hbar\omega$ is reached, whereas without them it is unaffected by temperature, indicating that the entire Fermi sea participates in the electronic transport.

Tunneling of electrons through classically forbidden regions is one of the major paradigms of quantum mechanics. Although our understanding has greatly improved over the past decades, some vital aspects of this process are still subject to fierce debates. For example, no consensus has been reached at yet whether so-called final-state blocking factors exist in the tunneling process across a barrier sandwiched between two conductors (Fig. 1), to enforce Pauli's exclusion principle that no two electrons may occupy the same quantum state. This seemingly innocent question is related to the question where in the so-called Fermi sea of conducting electrons the current actually flows, and thus has far-reaching consequences for our understanding of quantum transport. There are two schools on how to calculate the tunnel current, one that insists on using the blocking factors, and another that rejects them [1]. The dilemma is that both schools almost always seem to give identical answers for the current. In this Letter we point out that this result is fundamentally related to time-reversal symmetry, and study a generic system where this symmetry is broken to gain insight into the nature of blocking factors.

Consider a tunneling barrier impeding the current flow as depicted in Fig. 1. According to the first school, we start by calculating the *coherent* scattering states of the system consisting of an incident plane wave, a reflected wave, and a transmitted wave on the far side. These scattering states travel either from left to right or the opposite way. In the stationary limit they can simply be populated according to distribution functions f^{L} and f^{R} governing the asymptotic contact regions on either side. This yields for the current [1]

$$
\begin{aligned}
I_{\mathrm{S}} &= \frac{2e}{h}\int dE dE'\, \mathcal{D}_\perp T^{+}(E',E) f^{\mathrm{L}}(E) \\
&- \frac{2e}{h}\int dE dE'\, \mathcal{D}_\perp T^{-}(E,E') f^{\mathrm{R}}(E'), \qquad (1)
\end{aligned}
$$

where $\mathcal{D}_\perp$ is a density-of-states factor [2], $T^{+}(E',E)$ is the transmission probability for scattering states incident from the left at energy E and emerging at the right at E' ($\neq E$ in general), and T^{-} is defined in a similar manner for the reverse direction. According to Eq. (1) *all* scattering states contribute to the current, even those far below the Fermi surface — as recently discussed for the Fermi pump [3]. It is only when the transmission probabilities are symmetric, $T^{+}(E',E) = T^{-}(E',E)$, that the *net* current seems to stem from electrons in the immediate vicinity of the Fermi surface only, as in this case all electrons further down cancel each other.

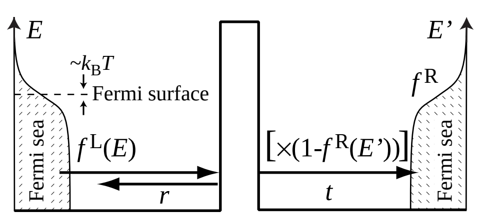

FIG. 1: Single-barrier scattering state with transmitted and reflected amplitudes, populated according to a distribution function f^{L} characterising the left side. In the Pauli picture, the tunneling probability incurs an additional final-state blocking factor $1 - f^{\mathrm{R}}$ on the right.

An alternative and widely used recipe for calculating the tunneling current in Fig. 1 is based on the transfer-Hamiltonian formalism, originally put forward by Oppenheimer [4], and later refined by Bardeen and others [5]. Here the system is split into two subsystems, the left- and the right-hand side, with a common overlap in the central barrier region, and the result for the current can be expressed as

$$
\begin{aligned}
I_{\mathrm{P}} &= \frac{2e}{h}\int dE dE'\, \mathcal{D}_\perp T^{+}(E',E)[1 - f^{\mathrm{R}}(E')] f^{\mathrm{L}}(E) \\
&- \frac{2e}{h}\int dE dE'\, \mathcal{D}_\perp T^{-}(E,E')[1 - f^{\mathrm{L}}(E)] f^{\mathrm{R}}(E') \qquad (2)
\end{aligned}
$$

which differs from Eq. (1) by the Pauli blocking factors $1 - f$. These factors are introduced — more or less *ad hoc* — using the intuitive argument that an electron tunneling from one side to the other needs to find an empty final state on the far side to tunnel into [6].

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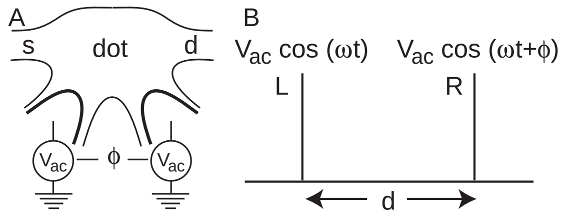

FIG. 2: Quantum-dot pump with broken time-reversal symmetry. [A] Schematic drawing; [B] simple 1D model based on driven δ-function barriers.

Clearly, the philosophies underlying Eqs. (1) and (2) are entirely different: For the former we assume that the left- and right-hand side of the barrier belong to the *same* system and that the scattering state extends coherently across the barrier, whereas in the latter we consider *real* incoherent transitions between initial and final states on opposite sides of the barrier belonging to *different* subsystems [7]. Both views have their merits. Certainly in the limit of a very transparent or even vanishing barrier, one has to regard both sides of the barrier as part of the same system, in which case there is no place for blocking factors. But equally well, if tunneling is weak, one can argue that the two sides do form two different subsystems, and that final-state blocking factors are mandatory to guarantee Pauli's exclusion principle and to prevent an "overflow" of the final state.

Crucially, this analysis also applies to a system with *local* time-dependent driving forces as its leads, and hence the distribution of incident electrons, are not affected by the driving field. For a system with time-reversal symmetry, it can be shown that the transmission probabilities are such that any channel $E \leftrightarrow E'$ is traversed with the same probability in either direction, i.e. that microreversibility holds, $T^+(E', E) \equiv T^-(E, E')$. Under this condition the cross terms $f^{\mathrm{L}} f^{\mathrm{R}}$ arising from the Pauli blocking factors cancel and Eqs. (1) and (2) yield identical answers for the *total* current, which is the quantity usually measured in experiment. It is probably because of this indecisive result that both schools have coexisted for so long. The only difference between the two is their prediction *where* in the Fermi sea the current flows: With blocking factors, the current is forced to flow close to the Fermi surface, as in this picture lower-lying final states are blocked, whilst in the formulation based on scattering states the current flows in the entire Fermi sea.

However, if time-reversal symmetry does not hold, Eqs. (1) and (2) yield different answers even for the *magnitude* of the current itself as the cross terms do not cancel any longer. This is very intriguing as it gives us hope to come closer to an experimentally verifiable answer regarding the existence of Pauli blocking factors.

Our analysis is inspired by a recent experiment by the Marcus group [8]. A semiconductor quantum dot with source and drain point contacts has two additional lateral gates to which ac voltages of relative phase ϕ are applied (see Fig. 2 A). Time-reversal symmetry is broken unless ϕ is an integer multiple of π. Averaging over different dot configurations, they measured fluctuations of the emf voltage generated between the source and drain contacts. Previous theoretical studies employed the concept of adiabatic pumping [9]. We take a complementary perspective and view the pump current (which exists even in the *absence* of any applied source-drain bias) as due to photon-assisted tunneling [10].

As a model system of a driven dot strongly coupled to its leads we consider two harmonically oscillating δ-function barriers of equal strength V_{ac} a distance d apart in a 1D potential, with a variable phase difference ϕ in the ac signals as depicted in Fig. 2 B [11]. This is a very simplified model of the Marcus pump, but nevertheless it turns out to exhibit many of its characteristic properties. For calculating the transmission probabilities $T(E', E)$ across the dot we take advantage of the fact that we can split this problem into two parts: If we know the transmission and reflection amplitudes for each barrier separately, we can use the Fabry-Perot method of raytracing known in optics to calculate the interference pattern due to multiple reflections between the barriers. As in optics the partial interference amplitudes can be summed up to all orders in a geometric series, yielding for the transmission amplitudes at the far side [12]

$$t \;=\; t^R (I - K)^{-1} Q t^L, \tag{3}$$

where $K = Qr^L Qr^R$ describes one full round trip of the electron between the two barriers L and R, starting and ending at the R barrier. Each round trip an electron at energy $E_n = E + n\hbar\omega$ picks up a phase factor $Q_n = \exp[i(k_n d + \theta)]$ consisting of two parts: The phase $k_n d$ incurred after travelling a distance d with wave vector $k_n = \sqrt{2mE_n}/\hbar$, and a fixed but unknown phase θ. This latter phase is introduced to account for the random changes in magnetic field and dot geometry employed in the experiment to perform ensemble averages. In general, the phase θ depends on the electron energy, but for simplicity we ignore this and assume θ to be equally distributed. Under this condition ensemble averaging simply means averaging over θ at the end of the calculation.

Due to the discreteness of the photon energy, electrons emerge on the far side of the barriers at energies differing from their original energy E by multiples of $\hbar\omega$: $E' = E + n\hbar\omega$, the so-called sidebands. Consequently, all amplitudes in Eq. (3) have to be interpreted as *matrices*, and the transmission probability takes the form $T(E', E) = \sum_n \tilde{T}_n(E)\delta(E + n\hbar\omega - E')$.

Before presenting numerical results for strong driving, it is instructive to study the weak-driving limit, which can be solved analytically. Defining $T_{\mathrm{e}}(k, \varphi) = \eta^2\,(k_0/4k)\,\cos^2[d(k_0 + k)/2 + \varphi/2]$ where $\eta = V_{\mathrm{ac}} k_0 / E_0$ is the dimensionless pump amplitude and k_0 the wave vector of the incident electron, we obtain for the transmission probabilities in the first three sidebands up to η^2 [13]

$$\tilde{T}_0^+(\phi, \theta) \;=\; 1 + T_{\mathrm{e}}(-k_1, -\phi) + T_{\mathrm{e}}(-k_{-1}, \phi)$$

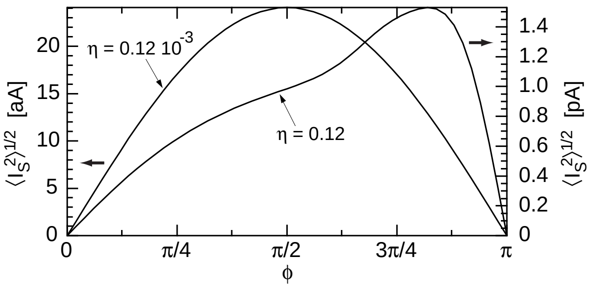

FIG. 3: Dependence of $\langle I_{\rm S}^2\rangle^{1/2}$ on the phase shift ϕ for weak and strong driving fields. Parameters: $d = 0.2\,\mu$m, $f = 10\,$MHz, $m = 0.067\,m_0$, $E_F = 12\,$meV, $T = 0.1\,$K.

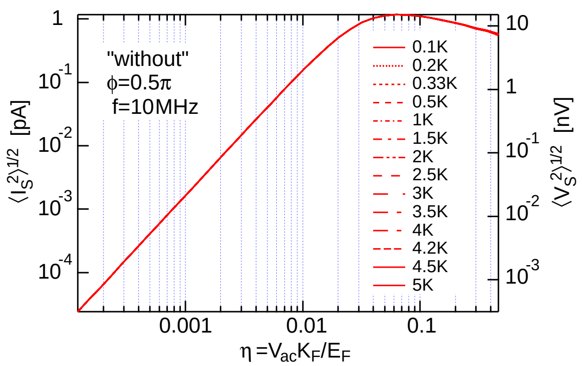

FIG. 4: $\langle I_{\rm S}^2(\pi/2)\rangle^{1/2}$ and $\langle V_{\rm S}^2(\pi/2)\rangle^{1/2}$, both based on Eq. (1), as a function of the driving strength $V_{\rm ac}$ for a range of temperatures.

$$\begin{aligned} & -T_{\rm e}(k_1, 2\theta-\phi) - T_{\rm e}(k_{-1}, 2\theta+\phi) \\ \tilde{T}^+_{\pm 1}(\phi,\theta) \;=\; & -T_{\rm e}(-k_{\pm 1}, \mp\phi). \end{aligned} \tag{4}$$

The corresponding transmission probabilities $\tilde{T}^-_n$ for the reverse direction are obtained by substituting $(\phi,\theta) \to (-\phi,\theta)$. As expected, the net transmission probability $\tilde{T}_{\rm net} \equiv \tilde{T}^+$ - $\tilde{T}^-$ vanishes for $\phi = n\pi$ when time-reversal symmetry holds, and is maximal at $\phi = \pi/2$. In agreement with experimental findings, the pump current at zero dc bias, being proportional to $\tilde{T}_{\rm net}$, scales with η^2 for weak driving. In the experiment the photon energy is 6 orders of magnitude smaller than the Fermi energy. Expanding Eq. (4) in this limit the current turns out to be *linear* in the driving frequency, in perfect agreement with the experimental results available [14].

After integrating over θ the ensemble average $\langle\tilde{T}_{\rm net}\rangle$ is found to be identically zero up to order η^2. This implies that the direct current $\langle I\rangle$ is orders of magnitude smaller than its fluctuations for all but the strongest driving fields, and hence we will concentrate on the mean square average $\langle I^2\rangle^{1/2}$ to study the fluctuations instead [15]. Figure 3 shows the dependence of $\langle I_{\rm S}^2\rangle^{1/2}$ on the phase shift ϕ, where we have used Eq. (3) with an adaptive number of photon sidebands to determine the full non-linear transmission probability, and Eq. (1) to finally calculate the current. For small driving amplitudes we find a $\sin\phi$ behaviour in agreement with Eq. (4), whilst for stronger driving nonharmonic features appear, both of which are in qualitative agreement with experiment. A similar behaviour is observed when using the formula (2) based on Pauli blocking factors instead, except that in this case the pump current is much smaller.

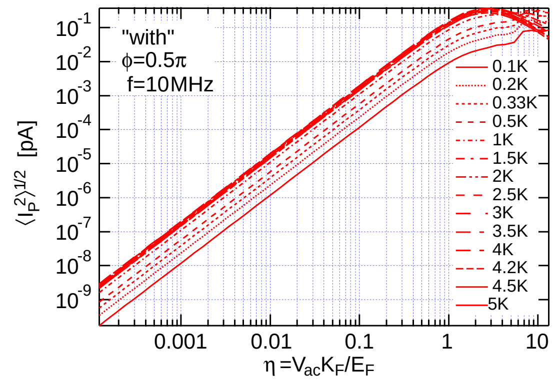

FIG. 5: $\langle I_{\rm P}^2(\pi/2)\rangle^{1/2}$, based on Eq. (2), as a function of the driving strength $V_{\rm ac}$ for a range of temperatures.

For the remainder of this Letter we will fix the ac phase shift ϕ to $\pi/2$, the point of maximal time-reversal asymmetry. The current fluctuations $\langle I_{\rm S}^2(\pi/2)\rangle^{1/2}$ calculated using the formula (1) *without* blocking factors are illustrated in Fig. 4 as a function of η, taken at the Fermi surface. For small driving amplitudes up to $\eta \approx 0.05$ the fluctuations increase quadratically with η as suggested by Eq. (4) before eventually starting to decrease. In the Marcus experiment, rather than measuring the pump current, the emf voltage generated was studied. Defining the emf voltage as the difference in chemical potentials between the left and right leads necessary to make the pump current vanish, we find that its fluctuations, also shown in Fig. 4 (right-hand axis), have virtually the same dependence on η as the current fluctuations. Both the quadratic rise as well as the levelling off for stronger pumping have been observed in experiment. The maximal emf fluctuations generated, 15 nV, is only one or two orders smaller than in the experiment, which is a quite reasonable agreement given the simplicity of the model.

The corresponding results based on the alternative formula (2) for the current which does include the Pauli blocking factors are illustrated in Fig. 5. Similar to the case without blocking factors of Fig. 4, the current fluctuations $\langle I_{\rm P}^2(\pi/2)\rangle^{1/2}$ (as well as the emf fluctuations, not shown) display an η^2 behaviour first before eventually starting to saturate. Yet, not only do the magnitudes of these results differ substantially from Fig. 4 for the same driving amplitude, but now there is a very pronounced temperature dependence as well!

This temperature dependence is worked out in more detail in Fig. 6 using a fixed driving strength of $\eta = 0.47$. Whilst without Pauli blocking factors the variation with temperature is minimal, an almost linear dependence is observed when they are included. This distinctly dif-

ferent behaviour in the low-temperature regime is most easily understood when looking at the number of states in phase space effectively available for transport: The blocking factors force the current to flow within a few $k_{\rm B}T$ of the Fermi surface (see Fig. 1), and as the temperature approaches zero, this range of active current-carrying states eventually diminishes to a minimal width of a few $\hbar\omega$, which in the experiment is much smaller than $k_{\rm B}T$. However, since each state can only carry a certain maximal load, it follows that the pump current must also decrease with temperature, until it settles for a residual value once $k_{\rm B}T \approx \hbar\omega$ is reached — with our parameters at $\approx 0.5\,$mK. On the other hand, without blocking factors there are no phase-space restrictions, in which case the pump current flows in the entire Fermi sea and thus is largely immune to changes at the Fermi surface brought about by temperature.

In the Marcus experiment the pump current is found to *increase* when lowering the temperature, and appears to level off at $\approx 0.1\,$K, where phase-breaking events become less important [8]. Such events are not included in our theory, and we can therefore not expect to reproduce the high-temperature behaviour. However, the experimental finding of a *saturated* pump current in the low-temperature limit is (if genuine and not due to thermal decoupling) only consistent with our results based on the scattering-state approach, Eq. (1), but *not* with the formulation relying on Pauli blocking factors, i.e. Eq. (2).

Being able to prove the (non)existence of Pauli blocking factors has drastic consequences for deciding whether the current flows in the entire Fermi sea or at its surface only. In this Letter we have demonstrated that a powerful tool for studying this issue is to look at the temperature dependence of the pump current when breaking time-reversal symmetry. Although our model system is simple, the conclusions about the low-temperature behaviour, being drawn from phase-space considerations, are clearly of a much more universal nature.

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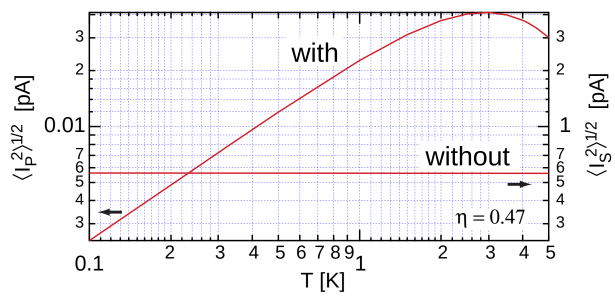

FIG. 6: Temperature dependence of $\langle I^2(\pi/2)\rangle^{1/2}$ with and without Pauli blocking factors.

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[13] Eq. (4) is almost identical to Eq. (4) of Ref. [11] which was derived within the WKB approximation, except for the fact that their result does not depend on the wave vector k_n of the outgoing channels. Summing over all channels n, Hekking *et al.* thus find the total transmission probability, in the absence of Pauli blocking factors, not to depend on the phase shift ϕ at all, and they conclude that there is no pump current in this case. This is, however, not a conclusive result, as it simply reflects their assumption of *unitary* total transmission probability even in the presence of the driving field.

[14] This linear relationship has been said to be a fingerprint of adiabatic pumping, but as seen here photon-assisted tunneling yields the same dependency.

[15] To avoid spurious low-energy resonance effects in the dot (which would not exist had we included potential fluctuations) we impose a lower cutoff to the energy integration in Eqs. (1) and (2) at 1 GHz. Changing this cutoff leads to small quantitative but no qualitative changes in our results.